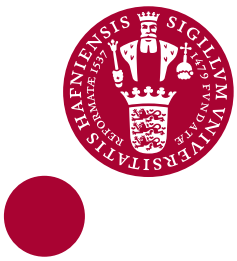

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Response to comment on 'Hydrogen bonds in crystalline D-alanine: diffraction and spectroscopic evidence for differences between enantiomers'

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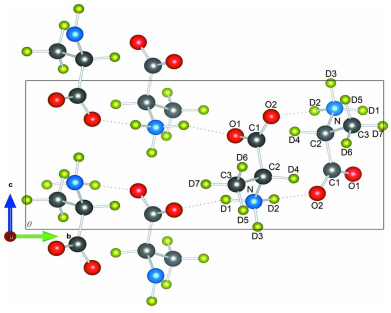
Keywords: chirality; structure analysis; configurational change; phase transitions; intermolecular interactions; amino acids.

In the preceding comment on our paper Bürgi & Macchi (2018) stated 'The recent paper by Belo, Pereira, Freire, Argyriou, Eckert & Bordallo [(2018), *IUCrJ*, **5**, 6–12] reports observations that may lead one to think of very strong and visible consequences of the parity-violation energy difference between enantiomers of a molecule, namely alanine' and 'Therefore, the conclusions drawn by Belo *et al.* (2018) are deemed inappropriate as the data presented do not contain sufficient information to reach such a conclusion'. In response to this comment we would like to stress the point that we did not in fact draw any conclusions at all in our paper concerning the parity-violating energy difference (PVED) hypothesis of Salam [Salam (1992), see also Laerdahl *et al.* (2000) and Berger & Quack (2000) for discussion] and therefore find it difficult to see how they could therefore be 'deemed inappropriate'.

Belo *et al.* (2018) reports a careful parametric (temperature-dependence) study of D-alanine by polarized single-crystal Raman spectroscopy and neutron powder diffraction and makes comparisons with results on both L- and D-alanine drawn from the literature. At temperatures where the structural information from the reported neutron powder diffraction measurements can be compared with previous single-crystal X-ray diffraction in L-alanine (Lehmann *et al.*, 1972; Destro *et al.*, 2008) and single-crystal neutron diffraction in L- and D-alanine (Wilson *et al.*, 2005), there is good agreement when the difference between hydrogenated and deuterated samples is taken into account. The results reported by Belo *et al.* (2018), however, provide a continuous picture of the temperature evolution of the bonds in D-alanine from 280 K down to 4 K, which shows that while the average structure is kept the same (no changes in space group) in D-alanine, as opposed to L-alanine, local symmetry changes are seen at lower temperatures. Furthermore, below 250 K, both L-alanine and D-alanine appear to undergo micro-conformational transitions resulting from a subtle rearrangement of the hydrogen-bond network. This temperature corresponds with that where bulk measurements (Barthès *et al.*, 2002, 2003; Wang *et al.*, 2000, 2002; Sullivan *et al.*, 2003) have observed anomalies that were indicative of a phase transition. Although it should be noted that Sullivan *et al.* (2003) were able to reduce this anomaly by re-growing their sample, it has been observed in a number of different samples prepared by different groups and should therefore be considered to be a real effect of as yet undetermined nature.

We note that the results of Belo *et al.* (2018) do not provide, or claim to provide, evidence for, or against, the Salam hypothesis, which predicted that quantum mechanical cooperative and condensation phenomena may give rise to a second-order phase transition below a critical temperature linking the transformation of D-amino acids to L-amino acids. An order of magnitude estimate by Salam (1992) indicated a transition temperature of ~250 K. The work of Belo *et al.* (2018) does not support the idea of the D-alanine (D-ala) → L-alanine (L-ala) transformation, but instead provides a microscopic picture of the alanine solids consistent with the other experimental measurements. The properties of L- and D-alanine, and the L- and D-amino acids in general, are a fascinating, and important, area of study for our understanding of nature, irrespective of whether they are related, or not, to the weak nuclear force and parity violation.



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